Interaction between hydroxyfullerene and water

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Experimental data showing the radical changes in the structure of water and other polar liquids when introducing small amounts (about ten thousandth of per cent by mass) of surface active nanoparticles have been recently published. Hydroxyfullerene is a proper object for quantum chemical modeling of interaction between activated carbon nanoparticle and water. At the same time hydroxyfullerene is of great interest because of its possible applications in medicine, for water disinfection and for polishing nanosurfaces.

The report contains the results of quantum-chemical modeling that allow making the conclusions concerning on the degree of nanoparticle influence on the structure of aqueous solutions. The calculations were carried out in the framework of ab initio and semiempirical methods of quantum chemistry using the software complex GAMESS [1,2]. At the first stage, the quantum-chemical investigation of the interaction of α-naphthol and β-naphthol molecules with water was carried out within various quantum-chemical models in order to estimate the error value, which can be resulted from the application of simplified methods with insufficient basis sets. Thus comparison of calculation results with experimental data demonstrates ab initio Hartree-Fock method in the basis 6-31G basis set provides qualitatively correct conclusion on hydrogen bond energies for systems considered.

The interaction energy between hydroxyfullerene and water depends on amount and locations of OH-groups in carbon cluster. Thus for complex $C_{60}[OH]_{10} \cdot 10H_2O$ with symmetry C_5 ab initio calculations demonstrate that the energy of interaction between nanoparticle $C_{60}[OH]_{10}$ and water molecule nearly twice as big as the interaction energy of water molecules in dimer. Introduction of a metal atom inside the carbon cage leads to increasing of interaction energy with a water molecule by 15%. The semiempirical research demonstrates that hydroxyfullerene molecule forms a stable complex in water, being surrounded with 6 layers of water molecules.

[1] Granovsky A.A. PC GAMESS version 7.1.5, http://classic.chem.msu.su/gran/gamess/index.html.
[2] Schmidt M.W.; Baldridge K.K.; Boatz J.A.; Elbert S.T.; Gordon M.S.; Jensen J.H.; Koseki S.; Matsunaga N.; Nguyen K.A.; Su S.; Windus T.L.; Dupuis M.; Montgomery *J. A. J. Comput. Chem.* **14**, 1347 (1993).